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***Abstract* - Molecular dynamics simulations are presented for the stopping of a charged ion in an electron gas. Full Coulomb collisional processes are included, and the resulting particle wake and energy deposition profiles are examined. The present study is extensible to multicomponent plasmas, for evaluating parameters like dE/dx, straggling, blooming, and energy splits.**

Charged particle stopping is a fundamental process in plasma physics, relevant to designs for controlled fusion and practical fusion energy. For example, the fast ignition [1] variant of inertial confinement fusion (ICF) heats dense hydrogen fuel with a high-energy particle beam via charged particle stopping. The peak temperature depends on the beam-target interaction, viz. how far the beam penetrates and how broadly it spreads out as it deposits energy. Uncertainties in beam stopping translate into large differences in predicted fusion yield. Once fusion begins, nuclear reactions produce fast alpha particles that further heat the fuel. Self-sustaining fusion burn or ignition in ICF again depends on charged particle stopping, in this case for random alpha particles.

Molecular dynamics (MD) simulations provide a ready means to study charged particle stopping; a projectile transfers energy and momentum by Coulomb scattering from surrounding plasma particles. We evaluate this long-range interaction by particle-particle particle-mesh (PPPM) method in a scalable implementation, ddcMD [2]. MD integrates the particle trajectories non-perturbatively, so it includes electrostatic interactions to all orders. MD results thus apply to both weak- and strong-coupling problems, including highly charged beam and impurity or dopant target atoms, so long as electrons are not bound and are non-degenerate.

A single charged projectile in an electron gas is studied here. This one component plasma (OCP) is a useful model for a neutral laboratory system as most energy from a fast projectile is deposited in the electrons. We employ a 2.6 MeV projectile of charge Z=-10, i.e. opposite charge from a Ne nucleus, with the neon mass. (Simple analytic stopping models give the same result for either sign of the charge, and the negative value avoids binding of the classical electrons,) The electron density (10^{20}cc) and temperature (1.088 eV) give Γ_{ee}=1. The system contains two million particles in a periodic cubic cell of length 2708 Å. The projectile trajectory is angled within the box to minimize finite size effects from neighboring periodic replicas.

For stopping, dE/dx, we can just monitor projectile trajectory and kinetic energy over the simulation. The trajectory is nearly straight-line over > 200 fs, during which the projectile loses 0.33% of its energy. We also obtain much more information, including the full wake disturbance generated in the plasma by the moving projectile. Stopping is physically mediated by precisely these charge- and current-density perturbations, so their details merit scrutiny.

Fig. 1 shows the charge density and energy transfer density of the target electron gas. The energy transfer field equals $\vec{F} \cdot \vec{j}$ over volume elements of the system, with $\vec{F} = -\nabla V_{Coul}(r)$ from the projectile Coulomb potential, and $\vec{j}$ the local current density induced by the moving projectile. (This result is post-processed, so we approximate the PPPM forces in the periodic cell with the $1/r^2$ Coulomb force between projectile and target.) This gives the rate of work performed by the projectile on the target. Formally, the integral of $\vec{F} \cdot \vec{j}$ over all space gives rate of energy loss, dE/dt, of the projectile, related to the stopping, dE/dx.

The major part of the particle wake can be seen in the top image. The close-up image shows the region of the target plasma which receives most of the energy from the stopping projectile. There are faint colored streaks or rays that correspond to individual scattered electrons. A time series shows these sporadic, individual, strong scattering events as well as interactions with collective, many-particle excitations in the target. Such time-dependent, random events contribute to departures from the average dE/dx and to random angular deflections of the projectile. These so-called straggling and blooming parameters affect the localization of energy deposition by charged particle beams.

The analyses that we perform here can be easily extended to multi-component target plasmas. Integration of $\vec{F} \cdot \vec{j}$ between particular species then reveals the energy split, the percentage of energy transferred to ions versus that transferred to electrons. Fusion yield is sensitive to this parameter through its effect on the predicted ion temperature.

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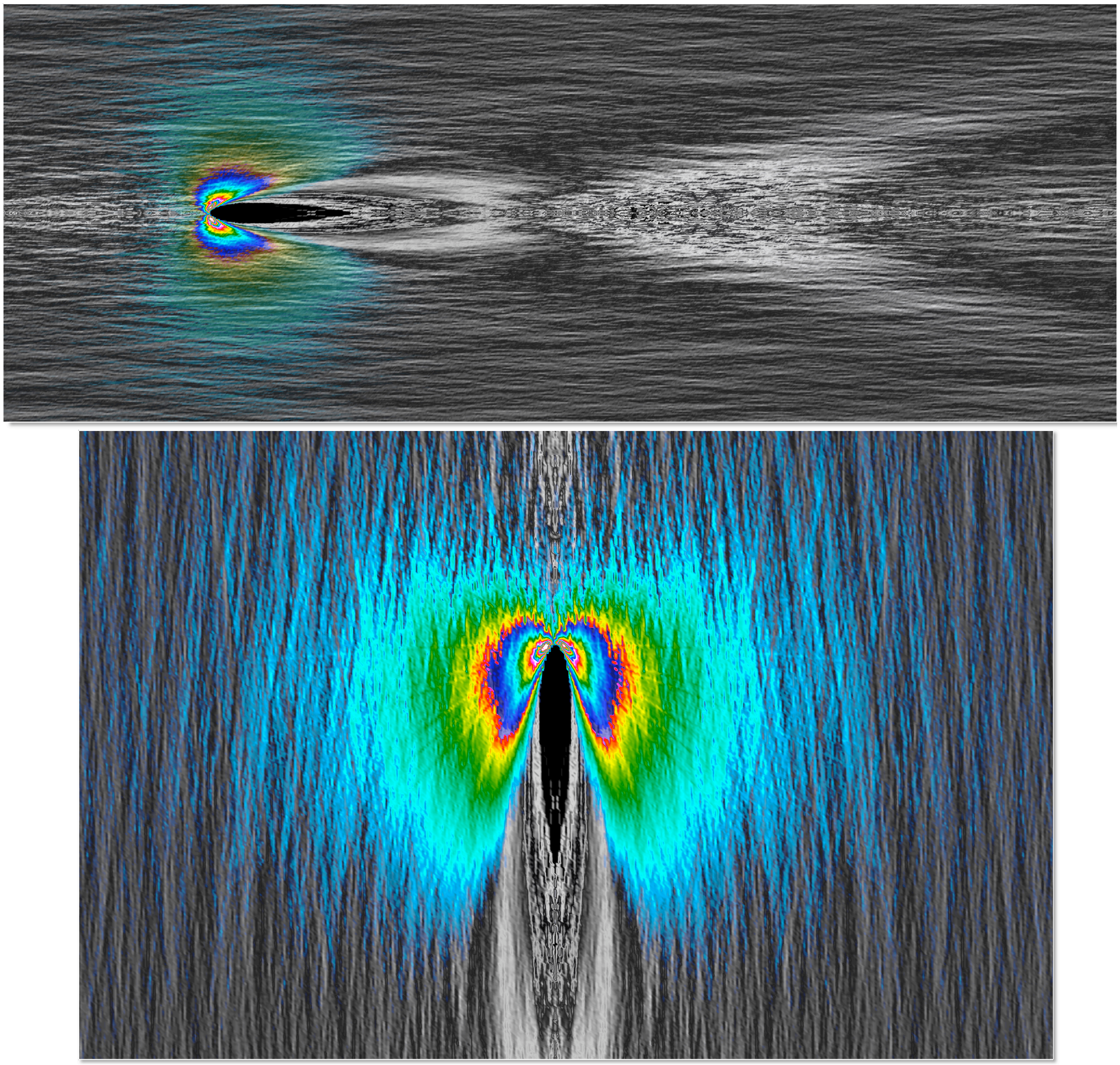

Fig. 1 The projectile wake field and the energy transfer field in the OCP are shown in gray scale and color, respectively. The top image spans 300 by 800 Å. The repulsive projectile is located towards the left side, moving left, in the tip of the dark ellipsoidal region with the wake trailing behind. The outer regions of the energy transfer density are made transparent in top view to show the underlying charge density. The energy flow is shown in greater detail in close-up, where the projectile is moving upwards. All fields are time- and rotationally-averaged (around the symmetry axis of the projectile velocity vector) to reduce statistical fluctuations. Residual density fluctuations are visible along the central axis (e.g. ahead of the projectile) because these cylindrical coordinates are averaged over smaller volumes.

REFERENCES

[1] M. Tabak, D. Hinkel, S. Atzeni, E.M. Campbell, and K. Tanaka, "Fast Ignition: Overview and background", Fusion Sci. and Tech. **49**, 254-277 (2006)

[2] D.F. Richards, J.N. Glosli, B. Chan, M.R. Dorr, E.W. Draeger, J.-L. Fattebert, W.D. Krauss, T. Spelce, F.H. Streitz, M.P. Surh, and J.A. Gunnels, "Beyond homogeneous decomposition,: scaling long-range forces on Massively Parallel Systems," Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis (2009)